Electronic Supplementary Material (ESI) for New Journal of Chemistry.

Supporting Information

Diaminomalenonitrile decorated cholesterol-based supramolecular gelator: Aggregation, multiple analytes (hydrazine, Hg^{2+} and Cu^{2+}) detection and dye adsorption

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Table 1S. Result of gelation test for compound **1**.

Solvent	**1**
DMSO	PS
DMF	S
CH_3CN	PS
CH_3OH	I
Toluene	PG
$CHCl_3$	S
Pet ether	PS
Cyclohexane	PS
Hexane	PS
DMSO : H_2O(1:1,v/v)	I
DMF : H_2O (1:1,v/v)	**G**
CH_3CN : H_2O (1:1,v/v)	I
DMF : CH_3OH (1:1, v/v)	S
Toluene : CH_3OH (1:1, v/v)	P
1,2-dichlorobenzene	**G**

S = solution; G = gel; PS = partially soluble; I = insoluble; PG = partial gel; P = Precipitation. Gelation tests were performed by taking 50 mg of the compounds in 1 ml of respective solvent.

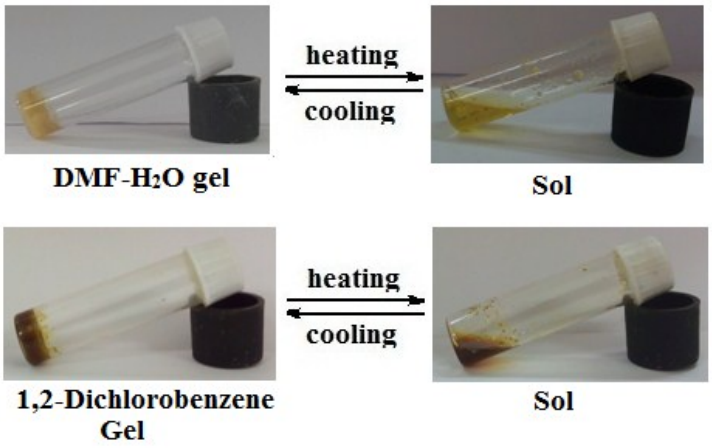


Fig. 1S. Pictorial representation of the thermoreversibility of the gels of **1** in DMF-H_2O (1:1, v/v) and 1,2-dichlorobenzene.

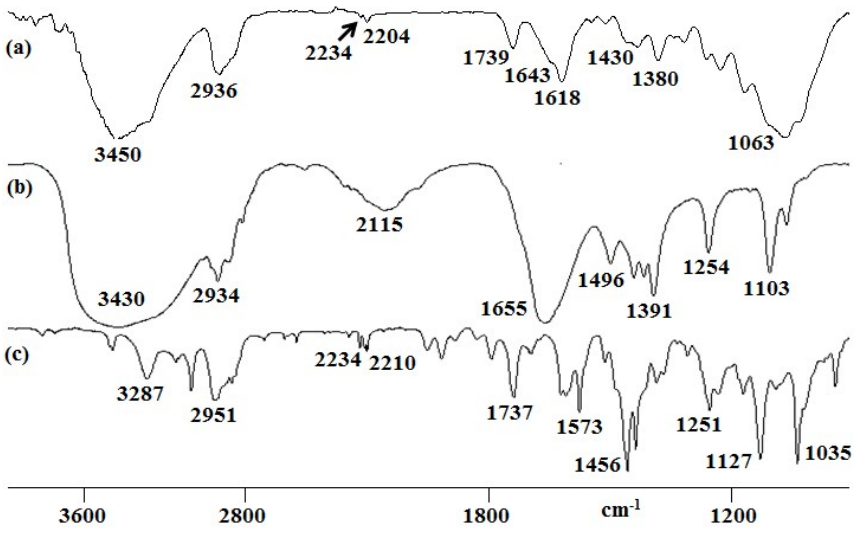


Fig. 2S. Partial FTIR spectra of **1** in (a) amorphous state and gel states in (b) DMF-H_2O (1:1, v/v) and (c) 1,2-dichlorobenzene.

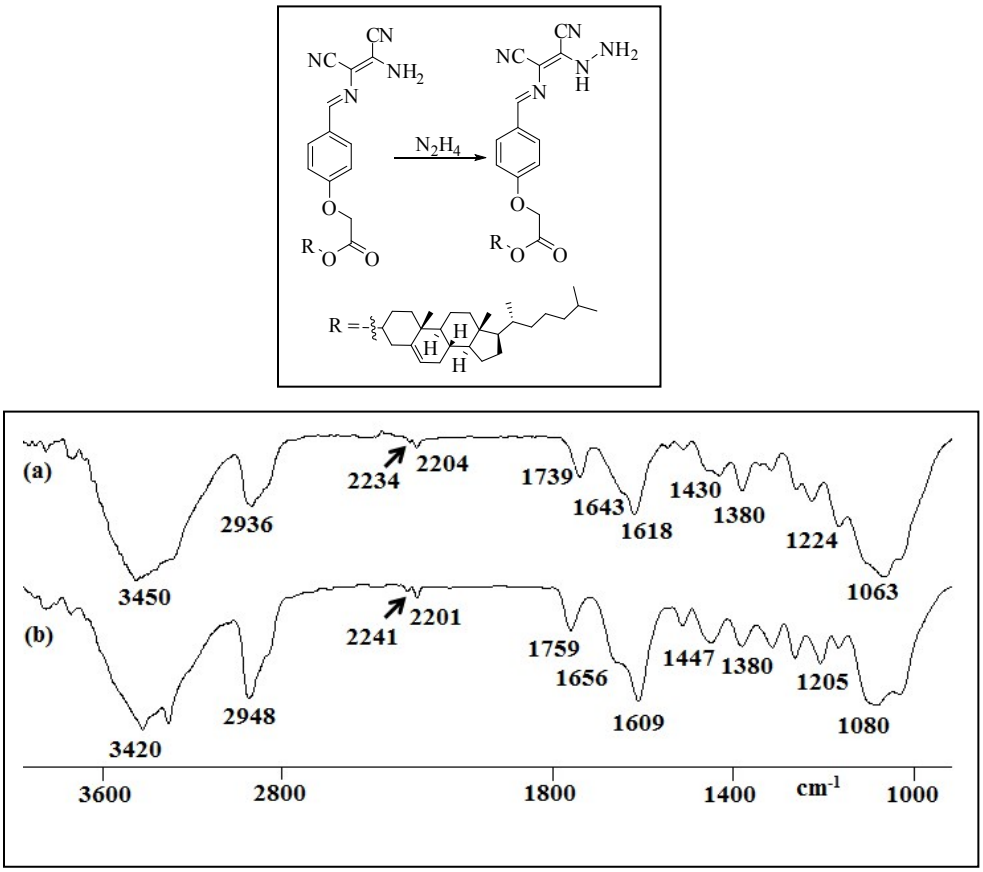


Fig. 3S. partial FTIR spectra of (a) **1** and (b) **1** with hydrazine

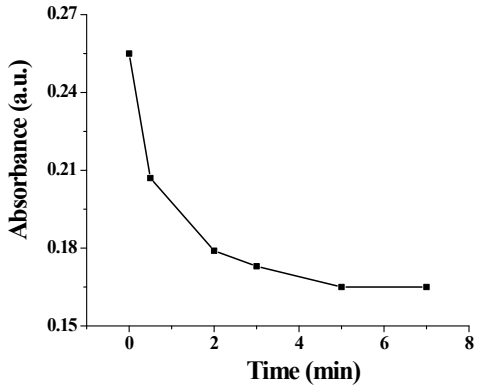


Fig. 4S. Change in absorbance of **1** (c = 2.50 x 10^{-5} M) with time in presence of equiv. amount of hydrazine (c = 1.0 x 10^{-3} M) at 323 nm.

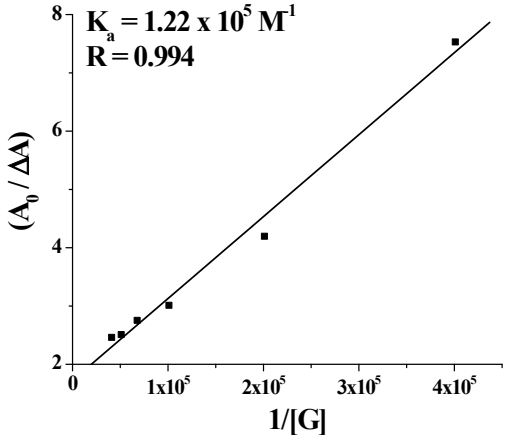


Fig. 5S. Benesi–Hilderband plot for **1** (c = 2.5 x 10^{-5} M) with hydrazine (c = 1.0 x 10^{-3} M) at 323 nm in DMF-H_2O (1:1, v/v).

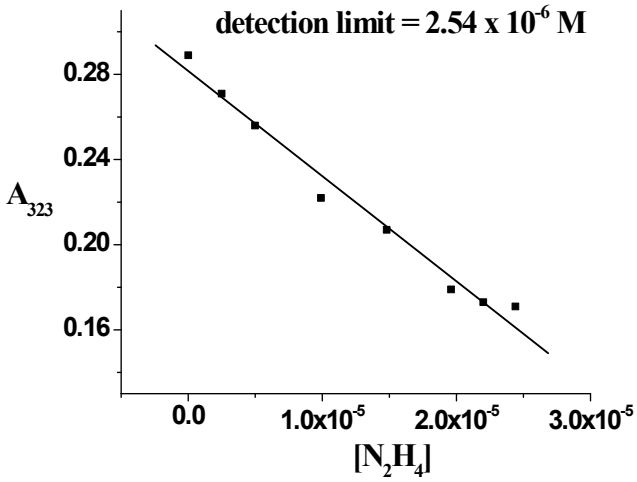
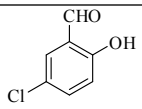
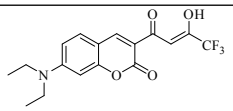
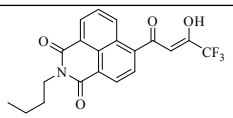
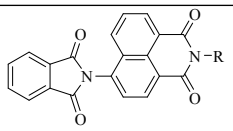
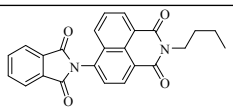
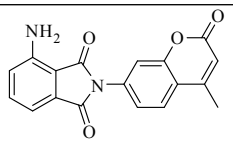
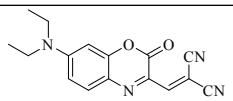
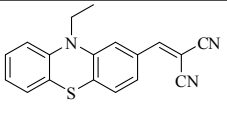
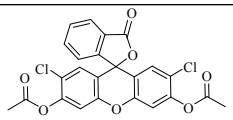
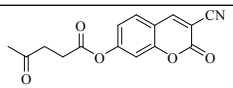
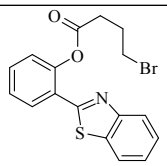
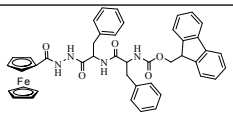
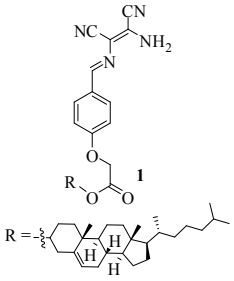


Fig. 6S. Detection limit of **1** (c = 2.5 x 10^{-5} M) with hydrazine (c = 1.0 x 10^{-3} M) at 323 nm in DMF-H_2O (1:1, v/v).

Table 2S: Reported structures for hydrazine sensing in solution phase.

Entry	Structure of compounds	Gel phase detection	Sensing mechanism	solvent	Detection limit (M)	Ref.
1		No	Fluorescence enhancement	ethanol/water/acetic acid = 30/66/4	8.0×10^{-8}	1
2		No	Ratiometric fluorescence response	CH_3CN	3.38×10^{-6}	2a
3		No	fluorimetric and colorimetric sensing	CH_3CN	1.0×10^{-7}	2b
4	 R = $(CH_2)_2O(CH_2)_2OH$	No	fluorimetric and colorimetric sensing	PBS buffer (pH 7.2, 10 mM) and EtOH (1:9, v/v);	4.2×10^{-9}	3a
5		No	fluorimetric and colorimetric sensing	DMSO-H_2O (6:4)	8.8×10^{-9}	3b
6		No	Colorimetric and ratiometric fluorescence sensing	H_2O/DMSO (3:7, v/v)	1.0×10^{-7}	3c
7		No	ICT-based ratiometric response	DMSO	7.0×10^{-10}	4a
8		No	Colorimetric and 'turn-on' fluorescence response	DMF–Tris. HCl buffer (10 mM, pH = 7.4, 7 : 3, v/v)	1.21×10^{-8}	4b

9		No	Fluorimetric and colorimetric sensing	DMSO - tris buffer (pH 8.0, 10 mM, 1 : 1, v/v)	9.0 x 10^{-8}	5
10		No	Colorimetric and 'turn-on' fluorescence response	acetate buffer (pH 4.5, 10mM) and DMSO (3:7, v/v)	2.65 x 10^{-6}	6
11		No	Ratiometric fluorescence response	CH_3CN:H2O (2:3, v/v, pH = 7.4, 1 mM HEPES buffer)	6.6 x 10^{-8}	7
12		yes	Indirect redox approach	Isopropanol – water (1 : 1, v/v)	-	8
Our work		Yes	Chemodosimetric approach Visual sensing through Gel-to-sol phase transition	DMF/H_2O (1:1, v/v)	2.54 x 10^{-6}	

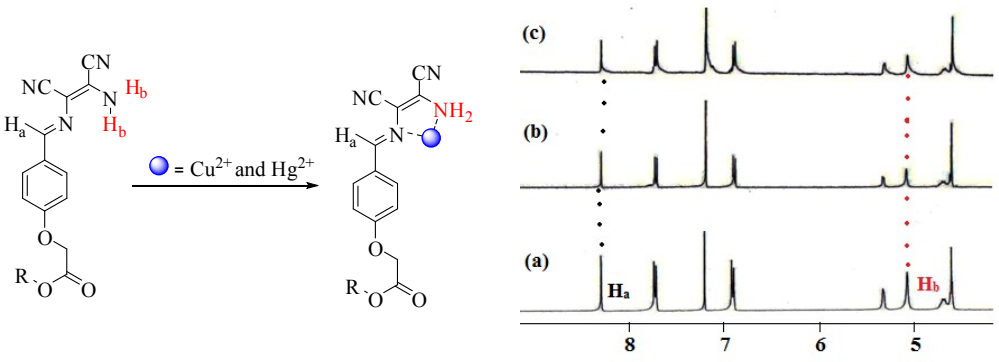


Fig. 7S. Partial ^{1}H NMR spectra of (a) **1** (c = 5.60 x 10^{-3} M), (b) 1 with Hg^{2+} (1:1, c = 0.05 M) and (c) 1 with Cu^{2+} (1:1, c = 0.02 M) in $CDCl_3$.

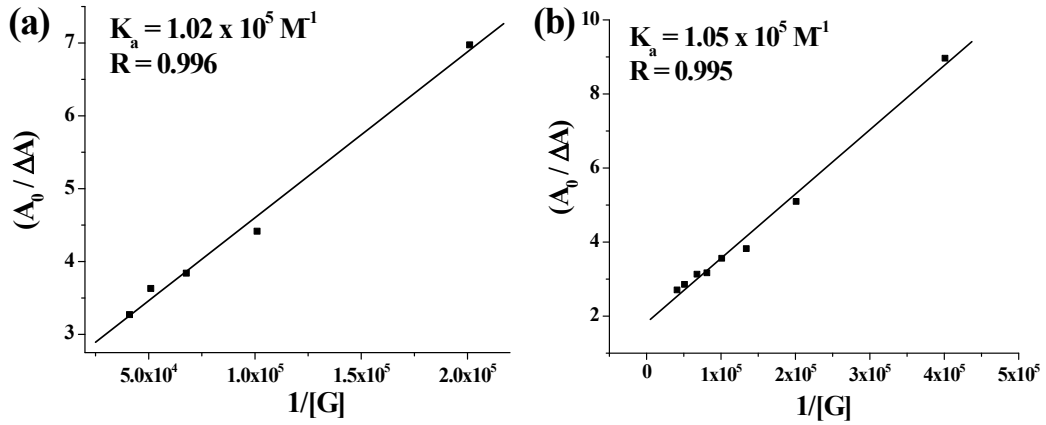


Fig. 8S. Benesi–Hilderband plot for **1** (c = 2.5 x 10^{-5} M) with (a) Hg^{2+} and (b) Cu^{2+} (c = 1.0 x 10^{-3} M) at 323 nm in DMF-H_2O (1:1, v/v).

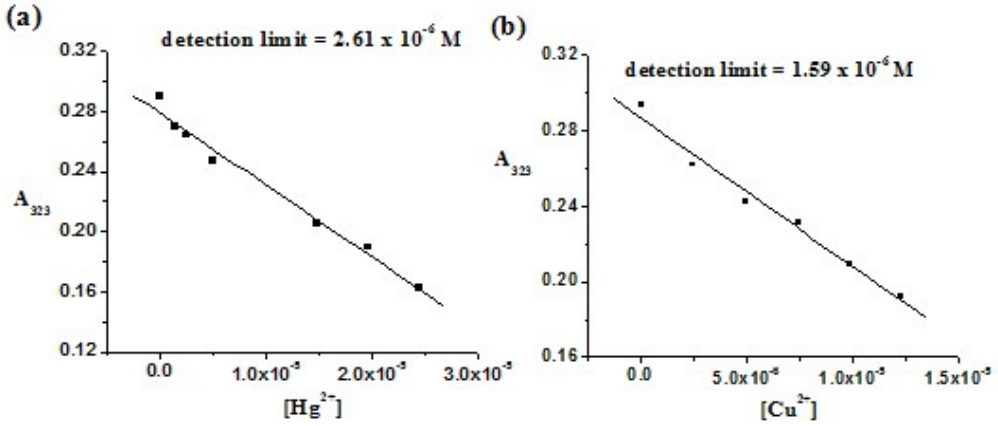
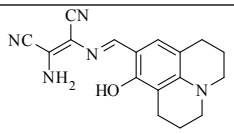
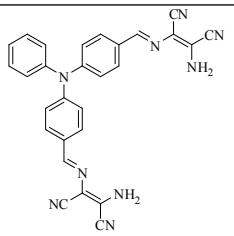
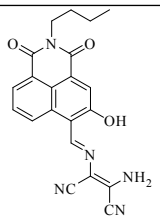
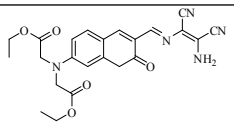
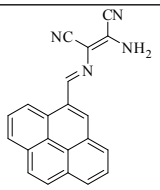
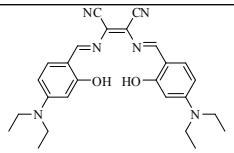
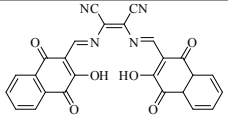
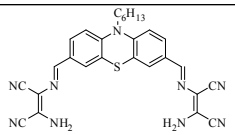
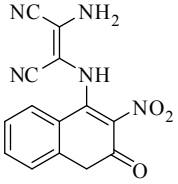
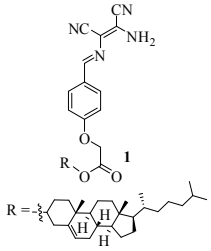


Fig. 9S. Detection limit of **1** (c = 2.5 x 10^{-5} M) with Hg^{2+} and (b) Cu^{2+} (c = 1.0 x 10^{-3} M) at 323 nm in DMF-H_2O (1:1, v/v).

Table 3S: Reported structures of diaminomalenonitrile based metal sensors

Entry	Structure of compounds	Sensing mechanism	solvent	Metal ion sense	Detection limit (M)	Ref.
1		colorimetric sensing	MeCN/bis-tris buffer (6 : 4, v/v)	Cu^{2+}	2.1 x 10^{-6}	9
2		ICT-based ratiometric response	H_2O:CH_3CN (1:1, v/v, pH 7.1)	Hg^{2+}	5.2 x 10^{-6}	10
3		colorimetric sensing	DMSO	Cu^{2+}	4.8 x 10^{-5}	11
4		colorimetric sensing	H2O/DMSO (v/v, 60/40)	Cu^{2+}	1.2 x 10^{-6}	12
5		Colorimetric and ‘turn-on’ fluorescence response	H_2O:CH_3CN (1:1, v/v, 10 mM HEPES, pH 7.0)	Cu^{2+}	-	13
6		Colorimetric and fluorescence response	CH_3CN	Cu^{2+}	4.9 ppb	14
7		colorimetric sensing	CH_3CN	Hg^{2+}	1.1 x 10^{-7}	15

8		Fluorimetric sensing	Ethanol-water (7:3)	Hg^{2+}	3.5×10^{-8}	16
9		colorimetric sensing	DMSO	Al^{3+}	3.82×10^{-5}	17
Our work		Visual sensing through Gel-to-sol phase transition	DMF/H_2O (1:1, v/v)	Hg^{2+} Cu^{2+}	2.61×10^{-6} 1.59×10^{-6}	

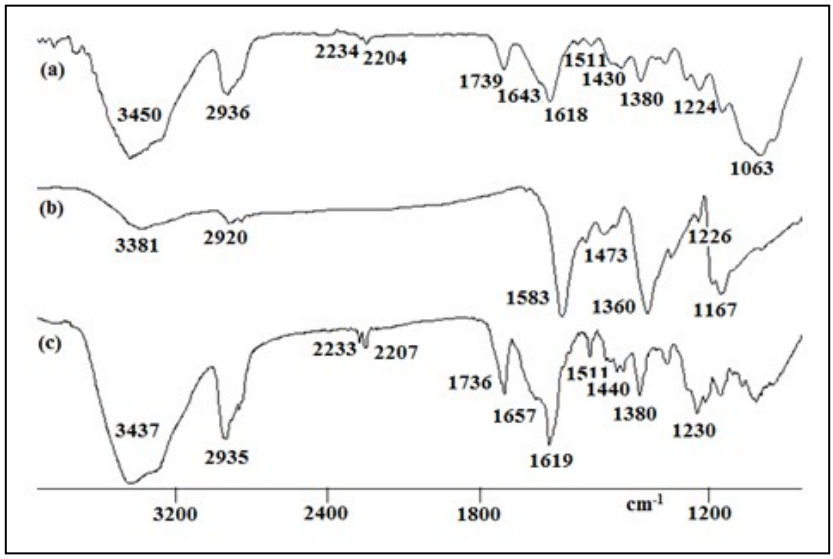
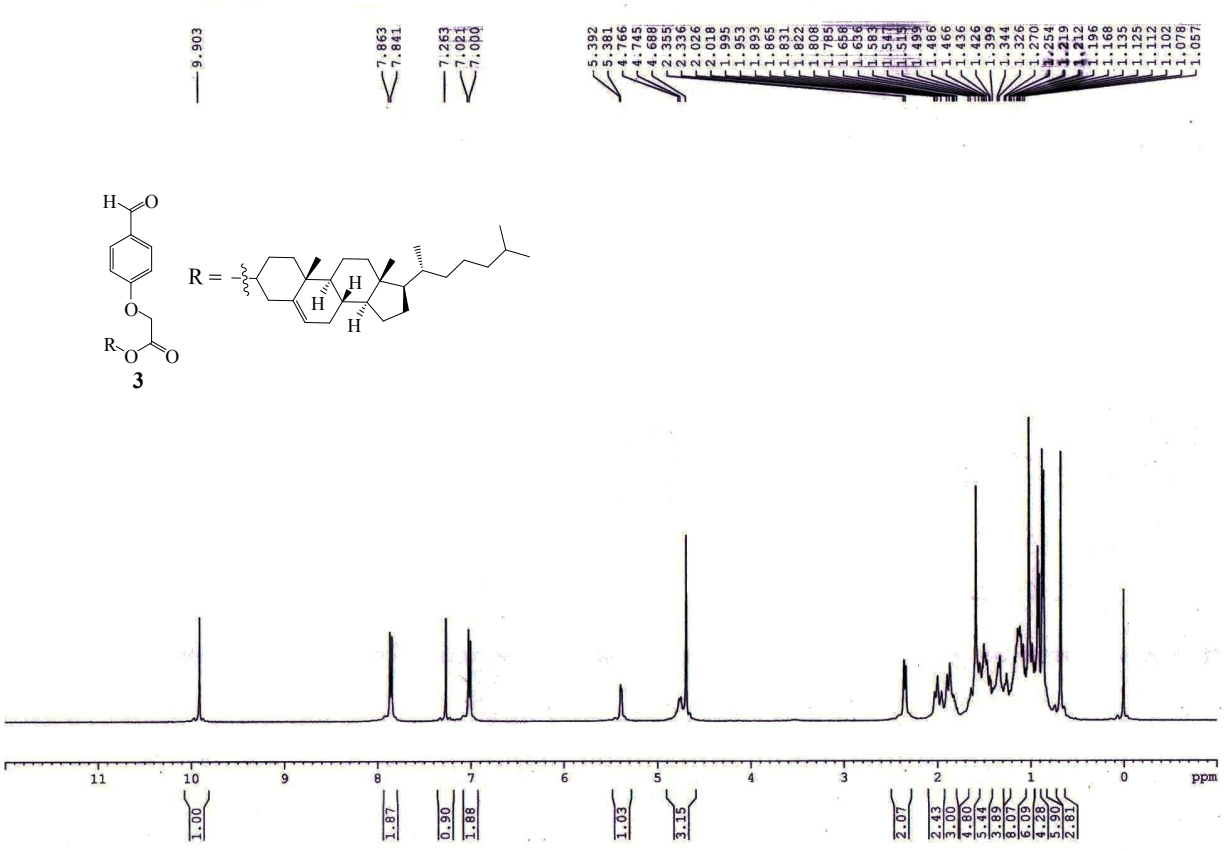
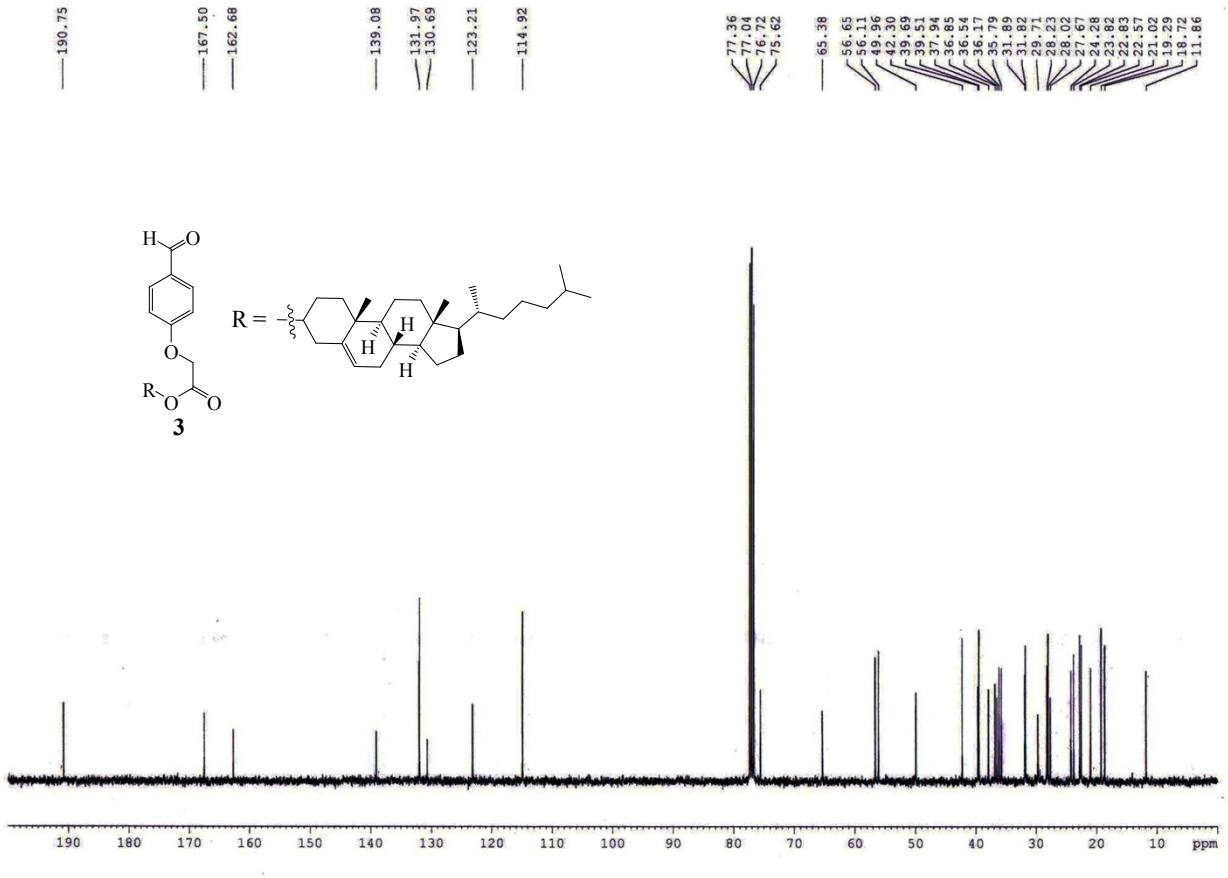


Fig. 10S. Partial FTIR spectra of (a) DMF-H_2O (1:1, v/v) gel of **1**, (b) Crystal Violet and (c) Crystal Violet adsorbed gel.

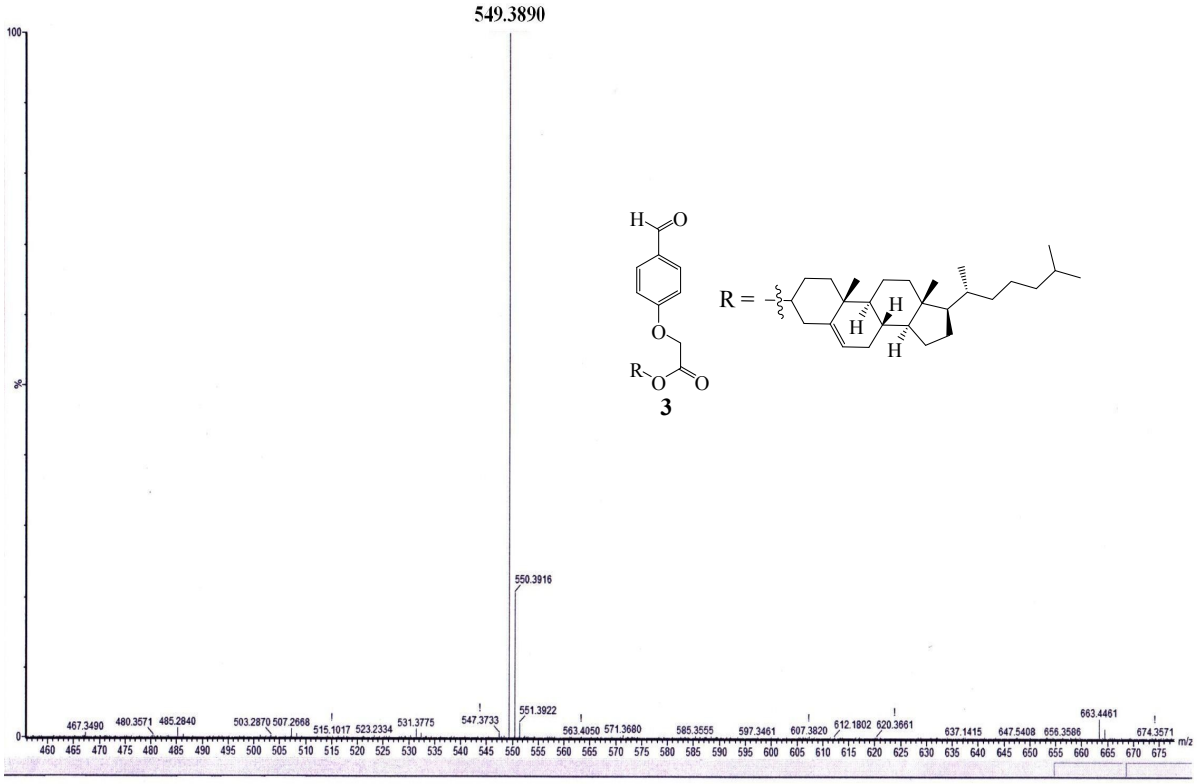
^{1}H NMR ($CDCl_3$, 400 MHz)



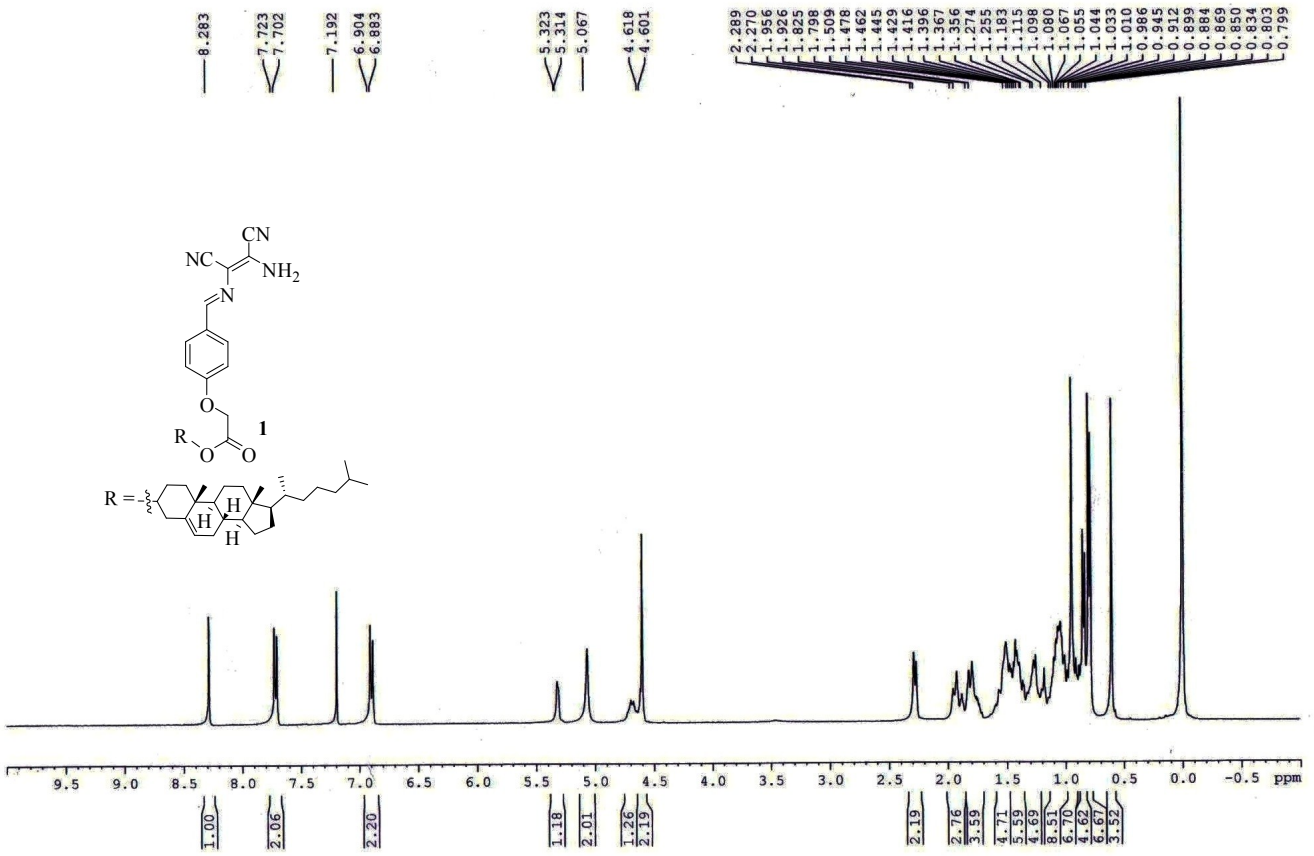
^{13}C NMR ($CDCl_3$, 100 MHz)



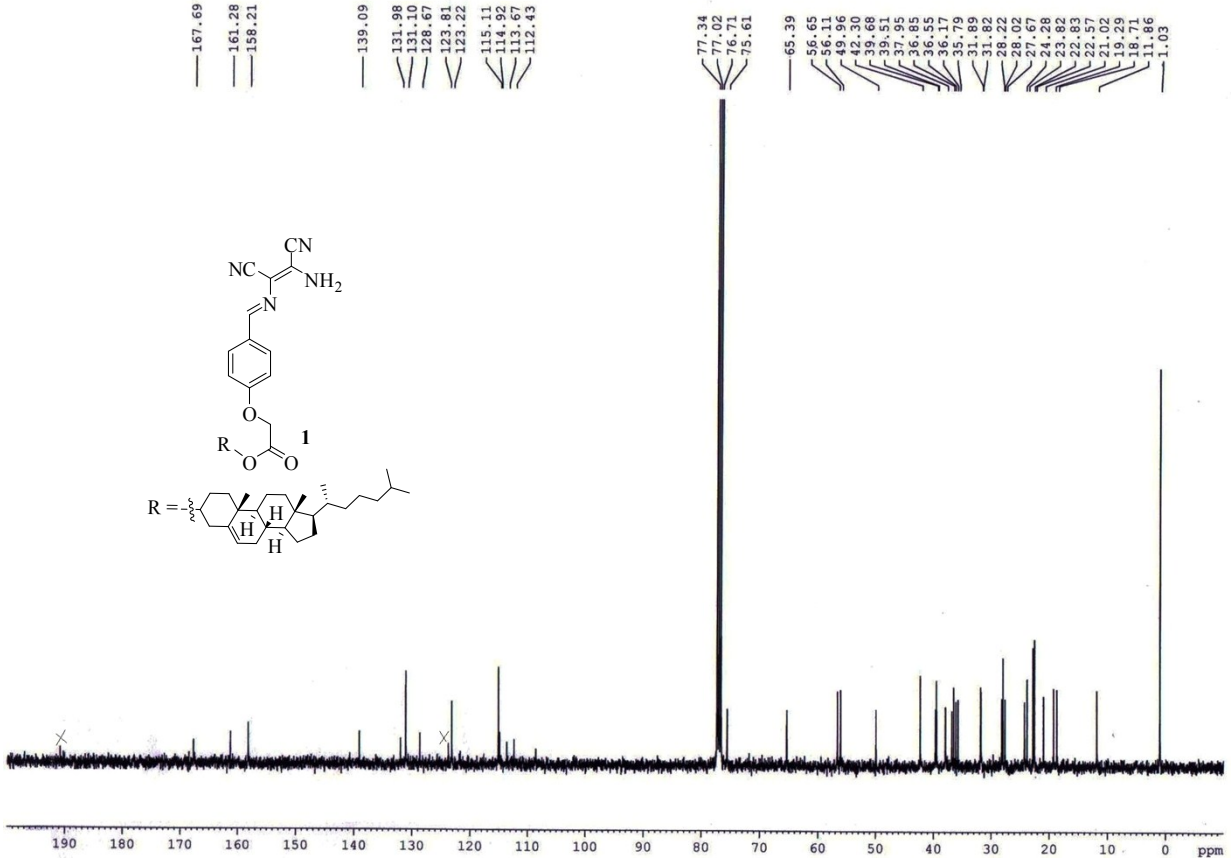
Mass spectrum of 3.



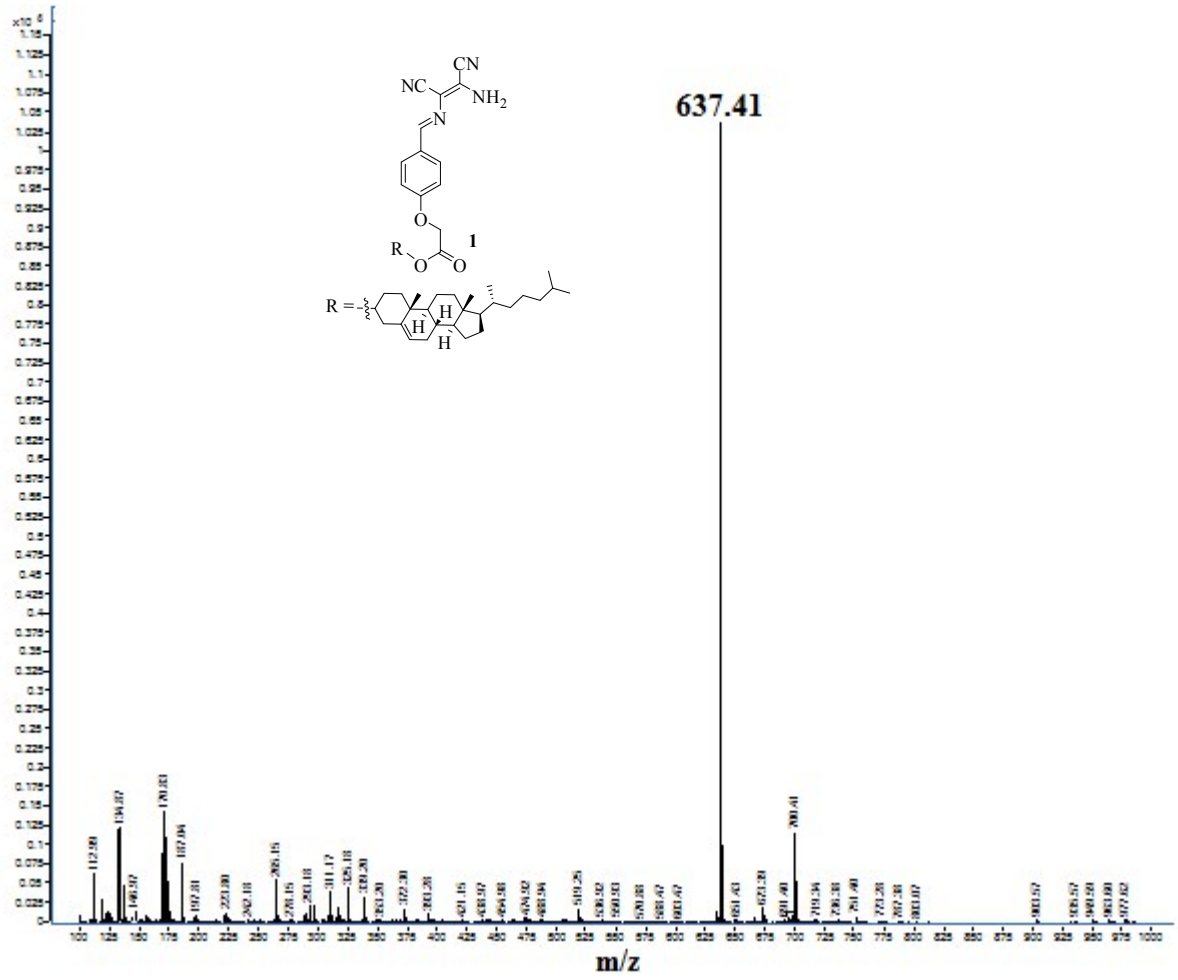
^{1}H NMR ($CDCl_3$, 400 MHz)



^{13}C NMR ($CDCl_3$, 100 MHz)



Mass spectrum of 1.



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